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NUMERICAL LINEAR ALGEBRA. (U)

AUG 81 G H GOLUB, J H WILKINSON

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FINAL SCIENTIFIC REPORT

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ABSTRACT

Research under this contract has been concentrated on major problems in numerical linear algebra. (i) The determination of error bounds for Gaussian elimination. (ii) The generalized eigenvalue problem $Ax = \lambda Bx$ and its natural extension to the computation of the canonical form of the pencil $A - \lambda B$ where A and B are $m \times n$ matrices. In addition, the numerical aspects of various problems in linear system theory and related fields have been studied.

RESEARCH REPORT

1. A Posteriori Error Bounds for Gaussian Elimination

Although in principle it has been known for many years how to derive error bounds for the solution of a system of linear equations calculated by Gaussian elimination, programs in this area have mainly been in machine code and on an ad hoc basis. Collaboration with F. W. J. Olver of the University of Maryland has led to the development of programs which can be coded in high level languages and should prove fully portable. They require no special hardware or software. The steps may be described in matrix terms by the following equations.

$$(i) \quad MA^{(n)} = A, \quad Mb^{(n)} = b. \quad (\text{Gaussian elimination})$$

M unit lower triangular; $A^{(n)}$ upper triangular

$$(ii) \quad VA^{(2n-1)} = A^{(n)}, \quad Vb^{(2n-1)} = b^{(n)}.$$

Here V is unit upper triangular and $A^{(2n-1)}$ is diagonal.

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MATTHEW J. KERPER

Chief, Technical Information Division

$$(iii) \quad A^{(2n-1)} x = b^{(2n-1)}$$

i.e. the solution of a diagonal system.

A backward error analysis is performed on each of these steps giving relations of the type

$$\bar{M}\bar{A}^{(n)} = A - \Delta A, \quad \bar{M}\bar{b}^{(n)} = b - \Delta b$$

where \bar{M} , $\bar{A}^{(n)}$ are the computed matrices and ΔA and Δb cover the rounding errors. For $|\Delta A|$ etc. we have only error bounds. For the determination of the error bounds we require the solution of the equations

$$\bar{L}\bar{M} = I \quad \text{and} \quad \bar{U}\bar{V} = I$$

and the error analysis of these processes gives for the computed matrices \bar{L} and \bar{U}

$$LM = I + \Delta L, \quad UV = I + \Delta U.$$

The use of these equations enables a bound to be found for $x - \bar{x}$.

The inherent errors in the data may be included in ΔA and Δb . The analysis provides for the possible use of lower precision arithmetic in the determination of \bar{L} and \bar{U} and in the computation of the error bounds themselves. This work is the subject of a joint paper (1) to be submitted for publication.

The collaboration with Olver, who had not previously worked in the linear algebra field, has been very productive for me. It came at a time when I was already interested in the problem of making research on rounding error analysis more readily accessible to non-specialists in the field, partly as a result of giving lectures in the Statistical-Numerical Analysis Summer Schools at Delaware (1980 and 1981). I am now convinced that rounding error analysis should be presented in an entirely different way. It was impractical to let this new approach influence the presentation in the joint paper with Olver but it will be the main thesis of a monograph on Rounding Error Analysis which is now in preparation. It is interesting that in many areas the whole

theory can be illustrated by means of examples with small integers in which the only errors are integer errors, so that no true rounding error analysis is involved. Hitherto the rather tedious detail associated with rounding errors has tended to obscure the underlying simplicity of what is being done and the underlying mathematical analysis is submerged.

J. H. Wilkinson

2. The Calculation of Error Bounds for Computed Eigenvalues and Eigenvectors and Invariant Subspaces

In practice it is rare for the complete eigensystem of a large matrix to be required. Commonly attention is focussed on a few key eigenvalues and eigenvectors. An algorithm is therefore desirable for deriving error bounds for a single eigenpair (i.e. value and vector) without requiring information on the remainder of the system. A method for deriving rigorous error bounds for such a pair λ and x was developed and has been published in Numerische Mathematik (2). A pleasing feature is that in the process of deriving the bounds an improved eigenpair is determined and the bound is for this eigenpair. The method covers both $Ax = \lambda x$ and $Ax = \lambda Bx$. In addition to a completely rigorous method a more practical technique is described which gives realistic bounds with far less computation.

A less pleasing feature is that the bound (and indeed, the true error) is limited by the condition number of a certain matrix C . The matrix C is ill-conditioned when λ is close to multiple roots. The latter are not necessarily ill-conditioned and hence this is an inherent weakness of the method.

This weakness has been overcome by determining generators of the invariant subspace associated with clusters of eigenvalues. This material was presented as an invited paper at an international symposium in honor of H. Rutishauser at ETH Zurich and has been published in the proceedings of the Symposium (3).

Although the algorithms described in the above two papers were essentially iterative they were designed to deal with initial approximations of high accuracy such as are provided by stable algorithms for solving the eigenvalue problem. Hence it was envisaged that only one of two iterations were required to obtain the limiting accuracy. Although they could be used for complex eigenvalues simply by working in complex arithmetic they were inefficient in dealing with complex conjugate pairs of eigenvalues of real matrices. In a third paper (4) resulting from collaboration with J. Dongarra of Argonne National Laboratory and C. Moler of the University of New Mexico extensions of the basic algorithm are described. These give (i) Quadratic convergence, efficiency being achieved in the iterations by an updating technique. (ii) Full efficiency for complex conjugate eigenvalues. (iii) Accurate generators of invariant subspaces associated with close clusters of eigenvalues whether or not they correspond to linear elementary divisors. Analyses of the influence of rounding errors on the performance of quadratically convergent algorithms are often based on unrealistic assumptions, mainly because of the tedious nature of the algebra involved. In a final section of this paper a program is described for performing this analysis on a computer, thereby making it a practical proposition to use a rigorous rounding error analysis.

J. H. Wilkinson

3. The Determination of the Distance of a Matrix from the Nearest Defective Matrix and the Corresponding Problem for $Ax = \lambda Bx$.

This is a problem of considerable interest to control engineers. Early work in connection with the standard problem was done by Kahan, Ruhe, and Wilkinson. The techniques developed by them have been greatly improved and extended to the generalized problem (the more important case). In the course of this work rather general results were derived which should be of considerable value in the backward error analysis of eigenvalue algorithms. This work was presented as an invited lecture at an international meeting held at the University of Manitoba and the paper (5) has been published in the proceedings.

Work has continued on problems associated with Kronecker's canonical form arising in control theory. Backward stable algorithms have been derived for computing Kronecker's canonical form and also the Drazin inverse. The techniques used in these papers are now being widely adopted. A summary of this work was presented at the 8th Gatlinburg meeting on Numerical Linear Algebra held at Oxford in July 1981; a full session at this meeting was devoted to the numerical problems arising in the control field.

J. H. Wilkinson

4. Application of the generalized Eigenstructure Problem in Linear System Theory

A new algorithmic approach was developed recently to tackle the generalized eigenstructure problem in its most general form. We applied these ideas to a set of specific problems. For each of them a numerical analysis of the problem was performed (6), (7), (8), (9), (10). Some algorithms were also implemented and tested (9), (10). The specific problems treated were:

- Computation of the controllable and unobservable subspaces, and of the Kalman decomposition.
- Computation of the supremal (A,B) -invariant subspace and (A,B) -controllability subspace in the kernel of C , computation of zeros (7),(9),(12).
- Construction and analysis of generalized state-space systems (7).
- Computing zeros of polynomial system models (6).
- Construction of cascade and spectral factorizations (8),(10).
- Solving Riccati equations arising in linear system theory (10).

Paul Van Dooren

5. Structural Properties and Sensitivity of Balanced Realizations

The robustness of certain properties (such as poles, zeros, observability, controllability, step response, etc.) of systems in state-space form depends highly on the chosen coordinate system. We analyzed the sensitivity of these properties for the so-called "balanced realization". The structural properties of balanced realizations for J -unitary transfer functions was investigated (8). Extensions for time-varying systems were considered (11). Possible implications for the synthesis of filters and predictors for "almost stationary" stochastic processes are under current investigations.

Paul Van Dooren

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- (1) F. W. J. Olver and J. H. Wilkinson, "A Posteriori Error Bounds for Gaussian Elimination." Submitted for publication.
- (2) H. J. Symm and J. H. Wilkinson, "Realistic Error Bounds for a Simple Eigenvalue and its Associated Eigenvector." Num. Math. 35 (1980) pp. 113-126.
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